Symmetries of Coincidence Site Lattices of Cubic Lattices

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Abstract

We consider the symmetries of coincidence site lattices of 3–dimensional cubic lattices. This includes the discussion of the symmetry groups and the Bravais classes of the CSLs. We derive various criteria and necessary conditions for symmetry operations of CSLs. They are used to obtain a complete list of the symmetry groups and the Bravais classes of those CSLs that are generated by a rotation through the angle π.

1 Introduction

Coincidence site lattices (CSL) are an important tool to characterize and analyze the structure of grain boundaries in crystals [1, 2]. At grain boundaries, two lattices with different orientation meet and it is thus natural to consider the intersection of these two lattices. Although grain boundaries are two–dimensional objects it proves useful to investigate the three–dimensional intersection of these two lattices [1, 2]. Usually those grain boundaries are preferred for which there is a high coincidence of lattice sites.

CSLs for three-dimensional cubic lattices have been investigated by various authors e.g. [3, 4, 5, 6, 7] and they are well understood. In particular one knows the coincidence rotations and has a handy parameterization for them, one knows the coincidence index Σ, the number of different CSLs for a given Σ, the generating functions, etc. Grimmer also discusses the equivalence classes [3] and some symmetry aspects of the CSLs [8, 9]. The latter is based on the computation of CSLs up to $\Sigma = 199$, but up to now systematic approaches to the symmetries of CSLs are rare and often unknown.[10]

In this paper we discuss the symmetries and the Bravais classes of CSLs. We start with recalling the basic notions and properties of CSLs. We review the equivalence classes of CSLs by using an approach that stresses the symmetry properties of the CSLs and that will prove useful in the determination of the symmetry groups of the CSLs. We then state some propositions on symmetry elements of CSLs in general and specialize them for three–dimensional cubic lattices. They enable us to determine the symmetry groups and Bravais classes for all CSLs that are generated by a rotation that is equivalent to a rotation through the angle π. Finally, we list all possible symmetry groups and Bravais classes for all three types of cubic lattices.

Let us fix some of the notations first. If m and n are integers, then $m|n$ means that m divides n. We shall use the following convention for vectors: 3–dimensional vectors will be characterized by an arrow, e.g. $\vec{r}$, whereas boldface letters denote 4–dimensional vectors and quaternions, e.g. $\boldsymbol{q}$. The corresponding inner (scalar) products will be written as $\vec{q}\cdot\vec{r}$ and $\langle\boldsymbol{q}|\boldsymbol{r}\rangle$, respectively. Furthermore $:=$ means "is defined by".

Let $\boldsymbol{L} \subseteq \mathbb{R}^n$ be an n-dimensional lattice and R a rotation. Then $\boldsymbol{L}(R) = \boldsymbol{L} \cap R\boldsymbol{L}$ is called a coincidence site lattice (CSL) if it is a sublattice[1] of finite index of $\boldsymbol{L}$, the corresponding rotation is called a coincidence rotation [7, 11]. The coincidence index $\Sigma(R)$ is defined as the index of $\boldsymbol{L}(R)$ in $\boldsymbol{L}$. By index we mean the group theoretical index of $\boldsymbol{L}(R)$ in $\boldsymbol{L}$, where we view $\boldsymbol{L}(R)$ and $\boldsymbol{L}$ as additive groups. Physically, the index $\Sigma(R)$ is the ratio of the volume of the (primitive) unit cells of the lattices $\boldsymbol{L}(R)$ and $\boldsymbol{L}$.

In the following, we specify $\boldsymbol{L}$ to be a cubic lattice; in particular, we assume $\boldsymbol{L} = \boldsymbol{L}_p = \mathbb{Z}^3$, i.e. a primitive cubic lattice. This is an important case since the results of the primitive cubic case can be easily extended to the face centered and body centered case. We will do this in the end. Thus for the moment $\boldsymbol{L} = \mathbb{Z}^3$. Then one can show that a rotation is a coincidence rotation if and only if it is a orthogonal matrix with rational entries [4, 6, 7].

Now any proper rotation in three–dimensional space can be parameterized by quaternions (Cayley's parameterization) [12, 13, 14, 15]:

$$R(\boldsymbol{r}) = \frac{1}{|\boldsymbol{r}|^2}\begin{pmatrix} \kappa^2+\lambda^2-\mu^2-\nu^2 & -2\kappa\nu+2\lambda\mu & 2\kappa\mu+2\lambda\nu \\ 2\kappa\nu+2\lambda\mu & \kappa^2-\lambda^2+\mu^2-\nu^2 & -2\kappa\lambda+2\mu\nu \\ -2\kappa\mu+2\lambda\nu & 2\kappa\lambda+2\mu\nu & \kappa^2-\lambda^2-\mu^2+\nu^2 \end{pmatrix}, \tag{1}$$

[1] We call $\boldsymbol{L}'$ a sublattice of $\boldsymbol{L}$ if $\boldsymbol{L}' \subseteq \boldsymbol{L}$ i.e. if $\boldsymbol{L}'$ is a subset of $\boldsymbol{L}$.

where $\boldsymbol{r} = (\kappa, \lambda, \mu, \nu)$ and $|\boldsymbol{r}|^2 = \kappa^2 + \lambda^2 + \mu^2 + \nu^2$. For the ease of the reader we have listed some typical rotations and their corresponding quaternions in Table 1. Thus the rational orthogonal matrices can be parameterized by integral quaternions, i.e. by quaternions with integral coefficients $\kappa, \lambda, \mu, \nu$. Note that we will call a quaternion an integer quaternion if it is an integral quaternion $(\kappa, \lambda, \mu, \nu)$ or the sum of an integral quaternion with the quaternion $1/2(1,1,1,1)$. We call an integral quaternion $\boldsymbol{r} = (\kappa, \lambda, \mu, \nu)$ primitive if the greatest common divisor of $\kappa, \lambda, \mu, \nu$ equals 1. If not stated otherwise every (integral) quaternion will be assumed to be a primitive quaternion.

Crystallographers may not be familiar with quaternions. Loosely speaking they are four dimensional vectors that can be multiplied in a nice way. You can view the quaternion $\boldsymbol{r} = (\kappa, \lambda, \mu, \nu)$ as the 2×2–matrix

$$\kappa\sigma_0 + \lambda\sigma_1 + \mu\sigma_2 + \nu\sigma_3, \tag{2}$$

where

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \sigma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \tag{3}$$

$$\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \tag{4}$$

which are just the well known Pauli matrices (up to a factor i). The inner product of two quaternions $\boldsymbol{q} = (\alpha, \beta, \gamma, \delta)$ and $\boldsymbol{r} = (\kappa, \lambda, \mu, \nu)$ is just the ordinary inner product of $\mathbb{R}^4$

$$\langle \boldsymbol{q} | \boldsymbol{r} \rangle := \alpha\kappa + \beta\lambda + \gamma\mu + \delta\nu. \tag{5}$$

In addition, for any quaternion $\boldsymbol{r}$ we define the conjugated quaternion by $\bar{\boldsymbol{r}} := (\kappa, -\lambda, -\mu, -\nu)$. For more details we have to refer to the literature [12, 13, 14]. Although we will use quaternions extensively in the following no knowledge of quaternions is necessary to understand most of the results. Those who are not interested in the mathematical details may skip the proofs and simply keep in mind that quaternions are a nice way to parameterize 3–dimensional rotations.

As a matter of fact $R(\boldsymbol{r})$ describes a proper rotation (i.e. $\det R(\boldsymbol{r}) = 1$ for all $\boldsymbol{r}$) with rotation axis $\vec{v}_0 = (\lambda, \mu, \nu)^t$ and the rotation angle φ given by

$$\cos\varphi = \frac{\kappa^2 - \lambda^2 - \mu^2 - \nu^2}{\kappa^2 + \lambda^2 + \mu^2 + \nu^2}. \tag{6}$$

In particular $\varphi = \pi$ for $\kappa = 0$.

$\boldsymbol{q}$	$R(\boldsymbol{q})$
$(1,0,0,0)$	1
$(0,1,0,0)$	$2 \;\; x,0,0$
$(0,0,1,0)$	$2 \;\; 0,y,0$
$(1,1,0,0)$	$4^+ \;\; x,0,0$
$(0,1,1,0)$	$2 \;\; x,x,0$
$(0,1,-1,0)$	$2 \;\; x,\bar{x},0$
$(0,0,1,1)$	$2 \;\; 0,y,y$
$(0,1,1,1)$	$2 \;\; x,x,x$
$(1,1,1,1)$	$3^+ \;\; x,x,x$
$(3,1,1,1)$	$6^+ \;\; x,x,x$
$(m,n,0,0)$	$\phi = \arccos\frac{m^2-n^2}{m^2+n^2}$, [100]
$(m,n,n,0)$	$\phi = \arccos\frac{m^2-2n^2}{m^2+2n^2}$, [110]
(m,n,n,n)	$\phi = \arccos\frac{m^2-3n^2}{m^2+3n^2}$, [111]
(κ,λ,μ,ν)	$\phi = \arccos\frac{\kappa^2-\lambda^2-\mu^2-\nu^2}{\kappa^2+\lambda^2+\mu^2+\nu^2}$, $[\lambda\mu\nu]$

Table 1: Quaternions and their symmetry operations: The table lists the symmetry operations for several typical quaternions. If the rotation is a crystallographic one, the standard crystallographic notation is used. For proper coincidence rotations (i.e. non-crystallographic) we state the rotation angle ϕ and the lattice direction of the rotation axis.

One can show that the coincidence index is given by $\Sigma(R(\boldsymbol{r})) = |\boldsymbol{r}|^2/2^\ell$, where ℓ is the maximal power such that 2^ℓ divides $|\boldsymbol{r}|^2$ (see e.g. [4, 6, 7]).

Finally we mention a nice representation of the lattice vectors of a CSL. To this end we define the vectors

$$\vec{r}^{(0)} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix}, \qquad \vec{r}^{(1)} = \begin{pmatrix} r_0 \\ r_3 \\ -r_2 \end{pmatrix},$$
$$\vec{r}^{(2)} = \begin{pmatrix} -r_3 \\ r_0 \\ r_1 \end{pmatrix}, \qquad \vec{r}^{(3)} = \begin{pmatrix} r_2 \\ -r_1 \\ r_0 \end{pmatrix}. \tag{7}$$

for a primitive quaternion $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$. These vectors $\vec{r}^{(i)}$ are lattice vectors of $\boldsymbol{L}(R(\boldsymbol{r}))$. Furthermore they are linearly dependent, in particular $r_0\vec{r}^{(0)} - r_1\vec{r}^{(1)} - r_2\vec{r}^{(2)} - r_3\vec{r}^{(3)} = \vec{0}$. On the other hand, the vectors $\vec{r}^{(i)}$ span $\mathbb{R}^3$, hence we can obtain a basis if we appropriately choose three of them. Thus any lattice vector $\vec{v} \in \boldsymbol{L}(R(\boldsymbol{r}))$ is a rational linear combination of them. However, such a basis has two disadvantages. First, rational coefficients are not so handy as integer ones. Secondly there is no general rule on how to choose the three basis vectors and any choice would break the symmetry of the setting. These disadvantages can be avoided if we express the lattice vectors of $\boldsymbol{L}(R(\boldsymbol{r}))$ as integer combinations of more than three lattice vectors, which necessarily are linearly dependent. The following lemma states how this can be achieved and we will often refer to it later on:

Lemma 1.1 *The CSL $\boldsymbol{L}(R(\boldsymbol{r}))$ with $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$ is the $\mathbb{Z}$–span of the following vectors:*

- $\vec{r}^{(0)}, \vec{r}^{(1)}, \vec{r}^{(2)}, \vec{r}^{(3)}$ *if $|\boldsymbol{r}|^2$ is odd,*
- $\vec{r}^{(0)}, \vec{r}^{(1)}, \vec{r}^{(2)}, \vec{r}^{(3)}, 1/2\,(\vec{r}^{(0)} + \vec{r}^{(1)} + \vec{r}^{(2)} + \vec{r}^{(3)})$ *if $|\boldsymbol{r}|^2$ even but not divisible by 4,*
- $\vec{r}^{(0)}, 1/2\,(\vec{r}^{(0)} + \vec{r}^{(1)}), 1/2\,(\vec{r}^{(0)} + \vec{r}^{(2)}), 1/2\,(\vec{r}^{(0)} + \vec{r}^{(3)})$ *if $|\boldsymbol{r}|^2$ is divisible by 4.*

Proof: The CSL $\boldsymbol{L}(R(\boldsymbol{r}))$ with $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$ contains the vectors $\vec{r}^{(0)}, \vec{r}^{(1)}, \vec{r}^{(2)}, \vec{r}^{(3)}$,, see e.g. [7]. Hence the lattices $\boldsymbol{L}_i(\boldsymbol{r})$ generated by the vectors $\vec{r}^{(j)}, j \neq i$ are sublattices of $\boldsymbol{L}$ with index $r_i|\boldsymbol{r}|^2$ if $r_i \neq 0$. Let $\boldsymbol{L}'(\boldsymbol{r})$ be the $\mathbb{Z}$–span of $\vec{r}^{(i)}, i = 0, \ldots, 3$. Then $\boldsymbol{L}'(\boldsymbol{r})$ is a superlattice of $\boldsymbol{L}_i(\boldsymbol{r})$ and a sublattice of $\boldsymbol{L}(\boldsymbol{r})$). In order to determine the index of $\boldsymbol{L}'(\boldsymbol{r})$ in $\boldsymbol{L}$ we first observe $r_0\vec{r}^{(0)} - r_1\vec{r}^{(1)} - r_2\vec{r}^{(2)} - r_3\vec{r}^{(3)} = \vec{0}$. Thus we can express any vector $\vec{r}^{(i)}$ as a linear combination of $\vec{r}^{(j)}, j \neq i$ if $r_i \neq 0$. Since the r_i are relatively prime, $c\vec{r}^{(i)}, c \in \mathbb{Z}$ is an integer combination of $\vec{r}^{(j)}, j \neq i$ if and only if $r_i \big| c$. Hence $\boldsymbol{L}_i(\boldsymbol{r})$ is a sublattice of $\boldsymbol{L}'(\boldsymbol{r})$ with index r_i if $r_i \neq 0$, and hence the index of $\boldsymbol{L}'(\boldsymbol{r})$ in $\boldsymbol{L}$ is $|\boldsymbol{r}|^2 = 2^\ell \Sigma(R(\boldsymbol{r}))$. Furthermore $\boldsymbol{L}'(\boldsymbol{r})$ is a sublattice of $\boldsymbol{L}(R(\boldsymbol{r}))$ with index $|\boldsymbol{r}|^2/\Sigma(R(\boldsymbol{r})) = 2^\ell$. Thus $\boldsymbol{L}'(\boldsymbol{r}) = \boldsymbol{L}(R(\boldsymbol{r}))$ if $|\boldsymbol{r}|^2$ is odd. If $|\boldsymbol{r}|^2$ is even then $1/2\,(\vec{r}^{(0)} + \vec{r}^{(1)} + \vec{r}^{(2)} + \vec{r}^{(3)})$ is a vector of $\boldsymbol{L}(R(\boldsymbol{r}))$, and if $4\big||\boldsymbol{r}|^2$ then $\boldsymbol{L}(R(\boldsymbol{r}))$ contains all the vectors $1/2\,(v_i \pm v_j)$. Since none of these vectors is contained in $\boldsymbol{L}'(\boldsymbol{r})$, the claim follows. □

It follows from this lemma that every vector of the CSL can be written in the form $m_0\vec{r}^{(0)} + m_1\vec{r}^{(1)} + m_2\vec{r}^{(2)} + m_3\vec{r}^{(3)}$, where the coefficients m_i are integers or half integers, with the following constraints: If $|\boldsymbol{r}|^2$ is odd, all m_i must be integers, if $|\boldsymbol{r}|^2$ is even then the sum $\sum_{i=0}^{3} m_i$ must be an integer. An additional constraint applies if $|\boldsymbol{r}|^2$ is even but not divisible by 4. In this case $\boldsymbol{r}$ has exactly two odd and two even components. If the even components are r_{i_1} and r_{i_2} and the odd components are r_{i_3} and r_{i_4}, then $m_{i_1} + m_{i_2}$ (as well as $m_{i_3} + m_{i_4}$) has to be an integer, too. If we write $\boldsymbol{m} = (m_0, m_1, m_2, m_3)$ then these constraints can be summarized as follows: $\boldsymbol{m}$ has an even number of integral components and the product $\langle \boldsymbol{r}|\boldsymbol{m}\rangle$ is an integer. An equivalent condition is that $2|\boldsymbol{m}|^2$ and $\langle \boldsymbol{r}|\boldsymbol{m}\rangle$ are integers. Note that these coefficients m_i are not unique, since the vectors $\vec{r}^{(i)}$ are linearly dependent.

2 Equivalence classes of CSLs

Different coincidence rotations R may generate the same CSL or CSLs that are just rotated versions of each other, so that an appropriate notion of equivalence is desirable. Let G be the point group of the lattice $\boldsymbol{L}$. Then $\boldsymbol{L}(RQ) = \boldsymbol{L}(R)$ for all $Q \in G$. Moreover $Q'RQ$ generates a rotated copy of $\boldsymbol{L}(R)$, namely $\boldsymbol{L}(Q'RQ) = Q'\boldsymbol{L}(R)$ for all $Q', Q \in G$. These lattices are usually considered equivalent, since they are in a crystallographic equivalent orientation with respect to the lattice $\boldsymbol{L}$. So we say that two coincidence rotations R, R' are *equivalent* if there exist rotations $Q', Q \in G$ such that $R' = Q'RQ$. Some authors (e.g. Grimmer and Bollmann [3, 8, 2]) extend this definition and consider the lattices $\boldsymbol{L}(R)$ and $\boldsymbol{L}(R^{-1})$ as equivalent, too. This is well justified from the physicist's point of view, since $\boldsymbol{L}(R^{-1}) = R^{-1}\boldsymbol{L}(R)$ is a rotated copy of $\boldsymbol{L}(R)$. Nevertheless $\boldsymbol{L}(R^{-1})$ and $\boldsymbol{L}(R)$ are in general not in a crystallographically equivalent orientation with respect to $\boldsymbol{L}$, so we will use the more restrictive notion mentioned above throughout this paper. Note that both definitions coincide if $R^2 = 1$, i.e. if R is a twofold rotation or a mirror reflection.

It follows directly from the definition that the set of all coincidence rotations equivalent to R is the double coset GRG, i.e. the set of all rotations QRQ' with $Q, Q' \in G$. The determination of all equivalence classes of coincidence rotations is thus equivalent to the double coset decomposition of the group of all coincidence rotations $OC(\boldsymbol{L})$ with respect to the subgroup G. Let $H = H(R) = G \cap RGR^{-1}$. Then $HRG = RG$. If $G = \bigcup_i Q_i H$ is the coset decomposition

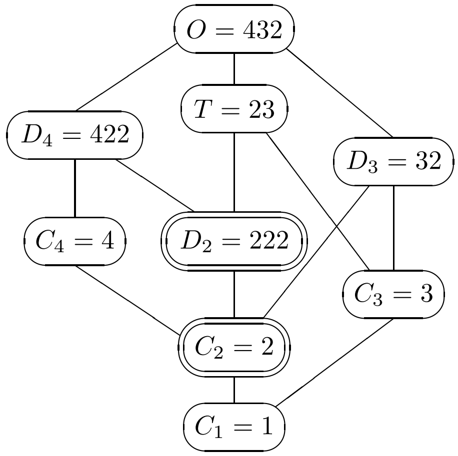

Figure 1: Subgroups of 432. Single circles are used if all subgroups of one type are conjugate under operations of 432, double circles indicate that the subgroups of these types are divided into two classes of conjugate subgroups. For instance, there exist nine different subgroups of type 2 corresponding to the nine rotations 2 of 432. Three of them are rotations about the cubic fourfold axes and the other ones are rotations about the cubic twofold axes. The fourfold axes are crystallographically equivalent directions, and so are the six twofold axes. Correspondingly we have two classes of conjugate subgroups of type 2, one class consisting of three subgroups and the other one consisting of six subgroups.

of G with respect to its subgroup H, then we can express the double coset GRG in terms of ordinary cosets $GRG = \bigcup_i Q_i RG$. Thus GRG consists of $|G|/|H|$ cosets, and hence the number of coincidence rotations equivalent to R is given by $|GRG| = |G|^2/|H|$ (see [16] for some more details on double cosets). Note that $H(R)$ and $H(R')$ are conjugated subgroups of G if R and R' are equivalent, in particular we have $H(R') = QH(R)Q^{-1}$ if $R' = QRQ'$.

We now turn to the three–dimensional cubic case. For simplicity, we restrict our considerations to proper rotations, i.e. $\det(R) = 1$ or $R \in SOC(\boldsymbol{L})$, where $SOC(\boldsymbol{L})$ denotes the group of all coincidence rotations R with $\det(R) = 1$. But this is no real restriction, since any improper rotation R' is equivalent to R if and only if $\bar{1}R'$ is equivalent to R, where $\bar{1}$ denotes the inversion. The group of all proper rotations leaving $\boldsymbol{L}$ invariant is $O = 432$ which is of order 24, the corresponding set of primitive quaternions consists of the 48 quaternions $(\pm1, 0, 0, 0)$, $(\pm1, \pm1, 0, 0)$, $(\pm1, \pm1, \pm1, \pm1)$ and permutations thereof. If these quaternions are normalized to unity, they form a group, too, namely the usual double cover[2] of O.

We have to determine the possible subgroups $H(R) \subset O$. Up to conjugacy, O has the following non trivial subgroups: the tetrahedral group 23 of order 12 generated by $3^+\ \ x, x, x$ and $2\ \ x, 0, 0$, the tetragonal group 422 of order 8 generated by $4^+\ \ x, 0, 0$ and $2\ \ 0, 0, z$, the tetragonal group 4 of order 4 generated by $4^+\ \ x, 0, 0$, the trigonal group 32 of order 6 generated by $3^+\ \ x, x, x$ and $2\ \ x, \bar{x}, 0$, the trigonal group 3 of order 3 generated by $3^+\ \ x, x, x$ and two orthorhombic subgroups 222 of order 4. One has the generators $2\ \ x, 0, 0$ and $2\ \ 0, y, 0$ and the other one has $2\ \ x, 0, 0$ and $2\ \ 0, y, y$, respectively. Finally there exist two monoclinic groups 2 of order 2 generated by $2\ \ x, 0, 0$ and $2\ \ x, x, 0$, respectively. Not all of them can be realized in the form $H(R) = O \cap ROR^{-1}$, e.g. the tetrahedral group is impossible. Fig. 1 shows these subgroups and the subgroup relations between them.

In order to determine the possible subgroups $H(R)$, it is convenient to know the classes of conjugated elements of O. They are well known (see e.g. [17]) and are the following: the unit element, the class of all rotations $3^\pm$ through $2\pi/3$, the class of all rotations $4^\pm$ through $\pi/2$, and two classes of rotations through π, namely $\{2\ \ x, 0, 0;\ 2\ \ 0, y, 0;\ 2\ \ 0, 0, z\}$ and $\{2\ \ x, x, 0;\ 2\ \ x, \bar{x}, 0;\ 2\ \ x, 0, x;\ 2\ \ x, 0, \bar{x};\ 2\ \ 0, y, y;\ 2\ \ 0, y, \bar{y}\}$.

Assume now that $H(R)$ contains the rotation $S = 3^+\ \ x, x, x$. Due to the definition of $H(R)$ the threefold rotation $R^{-1}SR$ is contained in O, too, i.e. it is a threefold rotation about the rotated axis $R^{-1}\vec{x}$, $\vec{x} = (1, 1, 1)$, which is parallel to one of the cubic threefold axis. Since all threefold axis are crystallographically equivalent there exists $Q \in O$ such that $R^{-1}\vec{x} = Q\vec{x}$, i.e. $R^{-1}SR = QSQ^{-1}$ or $R^{-1}SR = QS^{-1}Q^{-1}$. In the latter case we make use of $S^{-1} = TST^{-1}$, where $T = 2\ \ x, \bar{x}, 0$. We set $Q' = QT$ and get $R^{-1}SR = Q'SQ'^{-1}$. Thus there always exists an appropriate $Q \in O$ such that $R^{-1}SR = QSQ^{-1}$, in fact this is just a consequence of the well known fact that all threefold rotations are conjugate under operations of O. Equivalently we may write $SRQ = RQS$, and hence RQ commutes with S. Now RQ

[2]i.e. O is a homomorphic image of the corresponding group of quaternions and to each rotation there correspond exactly two normalized quaternions, i.e. $\boldsymbol{q}$ and $-\boldsymbol{q}$ correspond to the same rotation. This situation is well known from quantum mechanics, where a rotation through 2π changes the sign of the spinor and only a rotation about 4π leaves the spinor unchanged.

and S can commute only if their rotation axes are parallel and thus $RQ = R(m,n,n,n)$. Conversely $RQ = R(m,n,n,n)$ implies $S \in H(RQ) = H(R)$. It immediately follows from geometric intuition and it is straightforward to calculate that $3^+\ \bar{x},x,x \in H(R)$ would imply $RQ = R(1,1,1,1) = 3^+\ x,x,x$ for an appropriate $Q \in O$, and hence $H(R) = O$, so that the tetrahedral group cannot be realized as $H(R)$. Similarly one verifies that $2\ x,\bar{x},0 \in H(R)$ is possible if and only if $m = 0, \pm 1, \pm 3$ and $n = \pm 1$. This concludes the trigonal case.

One can proceed similarly if $S = 4^+\ x,0,0 \in H(R)$. Again R must map any rotation through $\pi/2$ onto a rotation of $\pi/2$, and since all these rotations are conjugated elements in O, there exists a $Q \in O$ such that RQ commutes with S, and this statement holds if and only if R is equivalent to $R(m,n,0,0)$. One shows again that if $H(R)$ contains an additional rotation about a twofold axis orthogonal to $(1,0,0)$, then $H(R) = O$. Thus the only group $H(R) \neq O$ that contains S is the tetragonal group generated by $S = 4^+\ x,0,0$.

It remains to check the orthorhombic and the monoclinic subgroups of O. It turns out that only the monoclinic group $H(R)$ with generator $2\ x,x,0$ can be realized, which is the case if and only if R is equivalent to $R(m,n,n,0)$, where $0 \neq |m| \neq |n| \neq 0$. These observations can be summarized as follows:

Theorem 2.1 *If R is equivalent to the sixfold rotation $R(3,1,1,1) \sim R(0,1,1,1)$, then the group $H(R)$ is conjugate to the trigonal group generated by $3^+\ x,x,x$ and $2\ x,\bar{x},0$ with $|H(R)| = 6$. Thus there are $4 \cdot 24$ (proper) rotations equivalent to $R(3,1,1,1)$.*

If R is equivalent to $R(m,n,n,n)$, $n \neq 0$, $m \neq \pm 3n$, then $H(R)$ is conjugate to the trigonal group generated by $3^+\ x,x,x$ of order $|H(R)| = 3$. There exist $8 \cdot 24$ equivalent (proper) rotations.

If R is equivalent to $R(m,n,0,0)$, $0 \neq |m| \neq |n| \neq 0$, then $H(R)$ is conjugate to the tetragonal group generated by $4^+\ x,0,0$ of order $|H(R)| = 4$. There are $6 \cdot 24$ equivalent (proper) rotations.

If R is equivalent to $R(m,n,n,0)$, $0 \neq |m| \neq |n| \neq 0$, then $H(R)$ is conjugate to the monoclinic group generated by $2\ x,x,0$. Its order $|H(R)| = 2$ and thus there are $12 \cdot 24$ equivalent (proper) rotations.

For all other $R \notin O$, we have $|H(R)| = 1$ and thus 24^2 equivalent (proper) rotations.

Number theory provides explicit expressions for the number of inequivalent rotations of the kind $(m,n,0,0)$, (m,n,n,n), and $(m,n,n,0)$. The number of representations of the binary forms m^2+n^2, m^2+3n^2, and m^2+2n^2 is well known and can be easily inferred from the prime decompositions of $\mathbb{Z}[i]$, $\mathbb{Z}[e^{2\pi i/3}]$ and $\mathbb{Z}[i\sqrt{2}]$, respectively [18, 15, 19]. The following theorem holds:

Theorem 2.2 *For given coincidence index Σ there are n_2 inequivalent rotations of the form $(m,n,0,0)$, n_3 rotations of the form (m,n,n,n) and n_4 rotations of the form $(m,n,n,0)$. The total number $f_{ineq}(\Sigma)$ of inequivalent rotations is given by*

$$f_{ineq}(\Sigma) = n_1 + n_2 + n_3 + n_4 + n_5, \tag{8}$$

where

$$n_1 = \begin{cases} 1 & \text{if } \Sigma = 3 \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

$$n_2 = \begin{cases} 2^{m-1} & \text{if } p = 1 \bmod 4 \text{ for all prime factors } p \text{ of } \Sigma \text{ and } m \text{ is the number of different prime factors of } \Sigma. \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

$$n_3 = \begin{cases} 2^{m-1} & \text{if } p = 1 \bmod 6 \text{ for all prime factors } p \neq 3 \text{ of } \Sigma > 3, \text{ the factor } p = 3 \text{ occurs at most once and } m \text{ is the number of different prime factors } p = 1 \bmod 6 \text{ of } \Sigma. \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

$$n_4 = \begin{cases} 2^{m-1} & \text{if } p = 1 \text{ or } 3 \bmod 8 \text{ for all prime factors } p \text{ of } \Sigma, \text{ where } m \text{ is the number of different prime factors of } \Sigma > 3. \\ 0 & \text{otherwise,} \end{cases} \tag{12}$$

and n_5 can be calculated from the total number of coincidence rotations $24f(\Sigma)$,

$$\begin{aligned} f(\Sigma) &= 4n_1 + 6n_2 + 8n_3 + 12n_4 + 24n_5 \\ &= \begin{cases} 0 & \text{if } \Sigma \text{ is even} \\ \Sigma \prod_j (1 + \frac{1}{p_j}) & \text{if } \Sigma \text{ is odd,} \end{cases} \end{aligned} \tag{13}$$

where the product runs over all prime factors of Σ.

For the last statement on the total number of coincidence rotations see [7, 8]. Note that $f(\Sigma)$ denotes the number of CSLs of index Σ.

3 Symmetries of CSLs

3.1 General remarks

We turn now to the question which symmetries the CSLs have, i.e. we want to find all rotations Q such that $Q\boldsymbol{L}(R) = \boldsymbol{L}(R)$ holds. For the moment, let $\boldsymbol{L}$ be an arbitrary lattice. Then $Q\boldsymbol{L}(R) = \boldsymbol{L}(R)$ is certainly satisfied if $Q \in G \cap RGR^{-1}$, where G denotes the symmetry group of $\boldsymbol{L}$. Furthermore R is a symmetry operation if $R^2 \in G$, i.e. in particular if $R^2 = 1$. This follows immediately from $R\boldsymbol{L}(R) = R\boldsymbol{L} \cap R^2\boldsymbol{L} = R\boldsymbol{L} \cap \boldsymbol{L} = \boldsymbol{L}(R)$ Thus, if R is a rotation through π, then R is a symmetry operation of $\boldsymbol{L}(R)$. Thus a CSL $\boldsymbol{L}(R)$ generated by a twofold rotation R has at least monoclinic symmetry. More generally, any rotation $Q \in RG$ such that $Q^2 \in G$ is a symmetry operation of $\boldsymbol{L}(R)$. Let us define

Definition 3.1 *The minimal symmetry group of $\boldsymbol{L}(R)$ is the group generated by $G \cap RGR^{-1}$ and all elements $Q \in RG$ such that $Q^2 \in G$.*

It is clear that the minimal symmetry group is a subgroup of the symmetry group of G. Naturally the question arises whether the symmetry group may contain additional elements, and we will see below that the answer is affirmative.

Let Q be a symmetry operation of $\boldsymbol{L}(R)$. Then $Q\boldsymbol{L}(R) = \boldsymbol{L}(R)$ implies

$$\boldsymbol{L}(R) = \boldsymbol{L} \cap R\boldsymbol{L} = \boldsymbol{L} \cap R\boldsymbol{L} \cap Q\boldsymbol{L} \cap QR\boldsymbol{L} \subseteq \boldsymbol{L} \cap Q\boldsymbol{L} = \boldsymbol{L}(Q). \tag{14}$$

Hence $|\boldsymbol{L}(Q) : \boldsymbol{L}(R)| \in \mathbb{N}$ and therefore Q must be a coincidence rotation such that $\Sigma(Q)$ divides $\Sigma(R)$. Similarly $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(QR)$ and $\Sigma(QR)\big|\Sigma(R)$. Conversely assume that $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(Q)$ and $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(QR)$ hold. Then $\boldsymbol{L}(R) \subseteq Q\boldsymbol{L} \cap QR\boldsymbol{L} = Q\boldsymbol{L}(R)$. Since Q is orthogonal we must have $\boldsymbol{L}(R) = Q\boldsymbol{L}(R)$, and hence Q is a symmetry rotation of $\boldsymbol{L}(R)$. We have thus proved

Theorem 3.1 *Q is a symmetry operation of $\boldsymbol{L}(R)$ if and only if $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(Q)$ and $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(QR)$ hold. If Q is a symmetry operation then Q is a coincidence rotation and $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(Q^nR^i)$ for all $n \in \mathbb{Z}$ and $i = 0, 1$. Thus $\Sigma(Q^nR^i)$ divides $\Sigma(R)$.*

The second part follows immediately from the first one since with Q also Q^n is a symmetry operation.

3.2 Symmetries of cubic lattices

3.2.1 Minimal symmetry groups

The minimal symmetry groups for a three–dimensional cubic lattice follow immediately from the preceding sections. Up to equivalence we have the following cases:

- The minimal symmetry group for $R = R(3, 1, 1, 1)$ is hexagonal and is generated by $R(3, 1, 1, 1)$ and $R(0, 1, -1, 0)$.
- If R is of the form $R(m, n, n, n)$, $0 \neq m \neq \pm n, \pm 3n \neq 0$, then the minimal symmetry group is trigonal and generated by $3^+ \;\; x, x, x$ and $R(0, n + m, n - m, -2n)$.
- If $R = R(m, n, 0, 0)$, $0 \neq m \neq \pm n \neq 0$, then the corresponding minimal symmetry group is tetragonal. The generators are $4^+ \;\; x, 0, 0$ and $R(0, 0, m, n)$.
- If $R = R(m, n, n, 0)$, $0 \neq m \neq \pm n \neq 0$ the minimal symmetry group is orthorhombic with generators $2 \;\; x, x, 0$ and $R(0, n, -n, m)$.
- If $R = R(0, \ell, m, n)$ is not equivalent to one of the cases above, then the minimal symmetry group is monoclinic and generated by R itself.
- If R is not equivalent to a rotation through π, then the minimal symmetry group is the trivial group consisting of the unit element only.

3.2.2 Further symmetry operations

Theorem 3.1 provides a criterion for symmetry operations. In order to make use of it we need the following lemma.

Lemma 3.2 *Let $\boldsymbol{q}$ and $\boldsymbol{r}$ be primitive. Then $\boldsymbol{L}(R(\boldsymbol{r})) \subseteq \boldsymbol{L}(R(\boldsymbol{q}))$ if there exists a (half)integral quaternion $\boldsymbol{m}$ such that $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$.*

Proof: Lemma 1.1 provides us with a very convenient representation of the lattice vectors of $\boldsymbol{L}(R)$, which we will use very often in the following. In Eq. (7) we have defined the vectors $\vec{r}^{(i)}$ for a quaternion $\boldsymbol{r}$, analogously we define $\vec{q}^{(i)}$ for a quaternion $\boldsymbol{q}$.

Now $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$ implies that $\vec{r} = m_0\vec{q} + m_1\vec{q}^{(1)} + m_2\vec{q}^{(2)} + m_3\vec{q}^{(3)}$, and according to the comments after lemma 1.1 we have $\vec{r} \in \boldsymbol{L}(R(\boldsymbol{q}))$ if both $2|\boldsymbol{m}|^2$ and $\langle \boldsymbol{q}|\boldsymbol{m}\rangle$ are integers. But this is certainly true since $r_0 = \langle \boldsymbol{q}|\bar{\boldsymbol{m}}\rangle$ is an integer. Similarly $\vec{r}^{(j)} \in \boldsymbol{L}(R(\boldsymbol{q}))$ follows from $\boldsymbol{r}\boldsymbol{u_i} = \boldsymbol{q}(\boldsymbol{m}\boldsymbol{u_i})$, where $\boldsymbol{u_i}$ are the unit quaternions $(0,1,0,0)$, $(0,0,1,0)$, and $(0,0,0,1)$, respectively. If $|\boldsymbol{r}|^2$ is odd, this proves the lemma. If $|\boldsymbol{r}|^2$ is even, then so is $|\boldsymbol{q}|^2$ or $|\boldsymbol{m}|^2$ (in the latter case $\boldsymbol{m}$ is integral). Hence $\langle \boldsymbol{q}|\boldsymbol{n}\rangle$ and $2|\boldsymbol{n}|^2$ are integers for $\boldsymbol{n} = 1/2\,(\boldsymbol{m}+\boldsymbol{m}\boldsymbol{u_1}+\boldsymbol{m}\boldsymbol{u_2}+\boldsymbol{m}\boldsymbol{u_3})$, which has again only (half)integral components, and thus $1/2\,(\vec{r}+\vec{r}^{(1)}+\vec{r}^{(2)}+\vec{r}^{(3)}) \in \boldsymbol{L}(R(\boldsymbol{q}))$. Similarly, one checks $1/2\,(\vec{r}^{(i)}+\vec{r}^{(j)}) \in \boldsymbol{L}(R(\boldsymbol{q}))$ if 4 divides $|\boldsymbol{r}|^2$. Thus all generators of $\boldsymbol{L}(R(\boldsymbol{r}))$ are in $\boldsymbol{L}(R(\boldsymbol{q}))$, which proves the lemma. □

In order to determine the symmetry group of the CSL $\boldsymbol{L}(R), R = R(\boldsymbol{r})$ it is sufficient to determine all twofold rotations that leave $\boldsymbol{L}(R)$ invariant. Thus we want to find all (primitive) quaternions $\boldsymbol{q} = (0, q_1, q_2, q_3)$ such that $Q = R(\boldsymbol{q})$ is a symmetry operation of $\boldsymbol{L}(R)$. In the following, we shall always assume that $\boldsymbol{q}$ is of the form $\boldsymbol{q} = (0, q_1, q_2, q_3)$.

First we state a simple result.

Lemma 3.3 *Let $\boldsymbol{r}$ and $\boldsymbol{q} = (0, q_1, q_2, q_3)$ be primitive quaternions. Then $Q = R(\boldsymbol{q})$ is a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$ if there exists a (half)integral quaternion $\boldsymbol{m}$ such that $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$ and $\boldsymbol{q}\boldsymbol{m} = -\boldsymbol{m}\boldsymbol{q}$ or $\boldsymbol{q}\boldsymbol{m} = \boldsymbol{m}\boldsymbol{q}$.*

Proof: According to lemma 3.2 we have $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(Q)$. Moreover $QR = R(\boldsymbol{m})$, and a second application of lemma 3.3 (maybe we have to shift a factor 2 from $\boldsymbol{q}$ to $\boldsymbol{m}$) gives $\boldsymbol{L}(R) \subseteq \boldsymbol{L}(QR)$, and hence by theorem 3.1 Q is a symmetry operation of $\boldsymbol{L}(R)$. □

The importance of this lemma lies in the fact that this exhausts more or less all cases for $\boldsymbol{r} = (0, r_1, r_2, r_3)$. The condition $\boldsymbol{q}\boldsymbol{m} = -\boldsymbol{m}\boldsymbol{q}$ implies that the real part of $\boldsymbol{q}$ and $\boldsymbol{m}$ vanishes, i.e. that $\boldsymbol{q}$ and $\boldsymbol{m}$ correspond to rotations through π, moreover the two rotation axes are orthogonal to each other. Corresponding CSLs have thus at least orthorhombic symmetry. The second case will be important in deciding whether a CSL with minimal trigonal symmetry is hexagonal or not.

We want to find some necessary conditions for symmetry elements Q. Since the vectors $\vec{r}^{(i)}$ are elements of $\boldsymbol{L}(Q)$ by theorem 3.1, we infer from lemma 1.1 that they can be written as $\vec{r}^{(i)} = n_0^{(i)}\vec{q} + n_1^{(i)}\vec{q}^{(1)} + n_2^{(i)}\vec{q}^{(2)} + n_3^{(i)}\vec{q}^{(3)}$, where the coefficients $n_j^{(i)}$ are integers or half-integers. If we define $\hat{R} = (\vec{r}, \vec{r}^{(1)}, \vec{r}^{(2)}, \vec{r}^{(3)})$ we can reformulate these equations as $\hat{R} = \hat{Q}N$, where the entries of the 4×4 matrix N are integers or half integers. But $\hat{R}$ can be obtained from $\pi(\boldsymbol{r})$ by skipping the first row, where π is the matrix representation of the quaternions defined by

$$\pi(1,0,0,0) = \tau_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{15}$$

$$\pi(0,1,0,0) = \tau_1 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{16}$$

$$\pi(0,0,1,0) = \tau_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \tag{17}$$

$$\pi(0,0,0,1) = \tau_3 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{18}$$

Thus $\pi(\boldsymbol{r}) = \pi(\boldsymbol{q})N + X$ for an appropriately chosen matrix

$$X = \begin{pmatrix} x_0 & x_1 & x_2 & x_3 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{19}$$

Hence there exists a (rational) quaternion $\boldsymbol{m}$ such that $N = \pi(\boldsymbol{m}) - \frac{1}{|\boldsymbol{q}|^2}\pi(\bar{\boldsymbol{q}})X$, explicitly

$$\begin{pmatrix} n_0^{(0)} & n_0^{(1)} & n_0^{(2)} & n_0^{(3)} \\ n_1^{(0)} & n_1^{(1)} & n_1^{(2)} & n_1^{(3)} \\ n_2^{(0)} & n_2^{(1)} & n_2^{(2)} & n_2^{(3)} \\ n_3^{(0)} & n_3^{(1)} & n_3^{(2)} & n_3^{(3)} \end{pmatrix} = \begin{pmatrix} m_0 & -m_1 & -m_2 & -m_3 \\ m_1 & m_0 & -m_3 & m_2 \\ m_2 & m_3 & m_0 & -m_1 \\ m_3 & -m_2 & m_1 & m_0 \end{pmatrix} + \frac{1}{|\boldsymbol{q}|^2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ q_1x_0 & q_1x_1 & q_1x_2 & q_1x_3 \\ q_2x_0 & q_2x_1 & q_2x_2 & q_2x_3 \\ q_3x_0 & q_3x_1 & q_3x_2 & q_3x_3 \end{pmatrix} \tag{20}$$

since $q_0 = 0$. Now $n_j^{(i)}$ are integer or half-integer and hence so are the m_i. Thus Q is a symmetry operation of $\boldsymbol{L}(R)$ only if there exists a (half) integral quaternion $\boldsymbol{m}$ such that $\boldsymbol{r} = \boldsymbol{qm}$. Since $\boldsymbol{r}$ is primitive, so is $2^\ell \boldsymbol{m}$, where $\ell = 0, 1$ according to whether $\boldsymbol{m}$ is integral or half integral. Thus we can state

Lemma 3.4 *The quaternion $\boldsymbol{q} = (0, q_1, q_2, q_3)$ corresponds to a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$ only if $\boldsymbol{m} := 1/|\boldsymbol{q}|^2\bar{\boldsymbol{q}}\boldsymbol{r}$ is a half integral quaternion.*

Note in passing that $2x_i$ is a multiple of $|\boldsymbol{q}|^2$ (since the q_i are relatively prime). Thus $N' = N + \frac{1}{|\boldsymbol{q}|^2}\pi(\bar{\boldsymbol{q}})X = \pi(\boldsymbol{m})$ is a (half)integer matrix and satisfies $\hat{R} = \hat{Q}N'$, too (remember that N is not uniquely defined).

We knew from lemma 1.1 and theorem 3.1 that $\vec{r}^{(i)}$ is an element of $\boldsymbol{L}(Q)$ and this has lead us to the representation $\boldsymbol{r} = \boldsymbol{qm}$. But we know even more about $\vec{r}^{(i)}$. If Q is a symmetry operation of $\boldsymbol{L}(R)$, then $Q\vec{r}^{(i)}$ and hence

$$\vec{r}^{(i)} + Q\vec{r}^{(i)} = \frac{2\vec{q}\cdot\vec{r}^{(i)}}{|\vec{q}|^2}\vec{q} = 2\bar{m}_i\vec{q} \tag{21}$$

are elements of $\boldsymbol{L}(R)$, where $\bar{m}_i$ are the components of the conjugate $\bar{\boldsymbol{m}}$ of $\boldsymbol{m}$. Since $2^\ell\boldsymbol{m}$ is primitive we infer $2^{1-\ell}\vec{q} \in \boldsymbol{L}(R)$. We are now in a similar situation as before. However, we do not know whether $2^{1-\ell}\vec{q}^{(i)} \in \boldsymbol{L}(R)$ or not, so we can only conclude that there exist a (half)integral quaternion $\boldsymbol{n}$ and an integer $x = \langle \boldsymbol{r}|\boldsymbol{n}\rangle$ such that $2^{1-\ell}\boldsymbol{q} = \boldsymbol{rn} - x\boldsymbol{e}$, where $\boldsymbol{e}$ is the unity quaternion. Expressing $\boldsymbol{q}$ in terms of $\boldsymbol{r}$ and $\boldsymbol{m}$ we get

$$\frac{2^{1-\ell}}{|\boldsymbol{m}|^2}\bar{\boldsymbol{m}} = \boldsymbol{n} - \frac{x}{|\boldsymbol{r}|^2}\bar{\boldsymbol{r}}. \tag{22}$$

This equation can hold only if $|\boldsymbol{q}|^2$ divides $2x = 2\langle \boldsymbol{r}|\boldsymbol{n}\rangle$, hence $y := \langle \boldsymbol{r}|\boldsymbol{n}\rangle/|\boldsymbol{q}|^2$ is integer or half integer. Now

$$|\boldsymbol{m}|^2|\boldsymbol{n}|^2 = 2^{2-2\ell} + y^2|\boldsymbol{q}|^2 \tag{23}$$

since $\langle \boldsymbol{r}|\boldsymbol{m}\rangle = 0$ due to $q_0 = 0$. But this implies that the greatest common divisor (=gcd) of $2|\boldsymbol{m}|^2$ and $|\boldsymbol{q}|^2$ is a power of 2, and so is and $\gcd(2|\boldsymbol{m}|^2, 2y)$. Hence $\Sigma(\boldsymbol{q})$ and $\Sigma(\boldsymbol{m})$ are relatively prime. Thus we have proved:

Theorem 3.5 *A twofold rotation $Q = R(\boldsymbol{q})$ can be a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$ only if there exists a (half) integral quaternion $\boldsymbol{m}$ such that $\boldsymbol{r} = \boldsymbol{qm}$ and $\Sigma(\boldsymbol{q})$ and $\Sigma(\boldsymbol{m})$ are relatively prime. In particular, if $\Sigma(\boldsymbol{r})$ is a prime power, then the symmetry group of $\boldsymbol{L}(R(\boldsymbol{r}))$ is just the minimal symmetry group.*

Next we want to have a closer look on Eq. (22). Since it is too difficult to discuss this equation in full generality we start with the case that $R(\boldsymbol{r})$ is a twofold rotation, i.e. $\boldsymbol{r} = (0, r_1, r_2, r_3)$. Let us further assume that $|\boldsymbol{q}|^2$ and $|\boldsymbol{r}|^2$ are both odd, hence $\boldsymbol{m}$ and $\boldsymbol{n}$ are integral quaternions. Thus

$$2\boldsymbol{m} = -y\boldsymbol{r} \bmod |\boldsymbol{m}|^2 \tag{24}$$

and in particular $2m_0 = 0 \bmod |\boldsymbol{m}|^2$. Hence $m_0 = 0$ or $2|m_0| \geq m_0^2$. The latter is satisfied only for the quaternions $(\pm 2, 0, 0, 0) \sim (\pm 1, 0, 0, 0)$, $(\pm 1, \pm 1, 0, 0)$ and permutations thereof. Since $\Sigma(\boldsymbol{m}) = 1$ for all of them, these are trivial solutions (if they are solutions at all), hence it remains to consider $m_0 = 0$. In this case $\boldsymbol{m}$ corresponds to a rotation through π, too, and the rotation axes $\vec{r}$, $\vec{q}$ and $\vec{m}$ must be mutually orthogonal. In particular the equations $\boldsymbol{r} = \boldsymbol{qm}$ and $\boldsymbol{q} = 1/|\boldsymbol{m}|^2\boldsymbol{r}\bar{\boldsymbol{m}}$ are equivalent to $\vec{r} = \vec{q} \times \vec{m}$ and $\vec{q} = (1/\vec{m}^2)\vec{m} \times \vec{r}$.

Similarly we can handle the case $|\boldsymbol{r}|^2$ odd and $|\boldsymbol{q}|^2$ even. Now $\boldsymbol{m} = 1/2\,\boldsymbol{m}'$, $\boldsymbol{m}'$ integral and $|\boldsymbol{m}'|^2$ even. $\boldsymbol{n}$ is again integral. Thus Eq. (22) reads

$$\boldsymbol{m}' = -2y\boldsymbol{r} \bmod |\boldsymbol{m}'|^2/2 \tag{25}$$

and we get the same trivial solutions (but now for $\boldsymbol{m}'$) as before, unless $2m_0 = m_0' = 0$. Thus again $\vec{r}$, $\vec{q}$ and $\vec{m}$ are orthogonal.

The case $|\boldsymbol{r}|^2$ even is slightly more difficult since $\boldsymbol{n}$ may be half integral now. Again we assume $|\boldsymbol{q}|^2$ odd first, hence $\boldsymbol{m}$ is integral and $|\boldsymbol{m}|^2$ is even but $4 \nmid |\boldsymbol{m}|^2$. We now replace condition (22) by the weaker condition

$$2\boldsymbol{m} = -y\boldsymbol{r} \bmod |\boldsymbol{m}|^2/2. \tag{26}$$

The only possible solutions for $\boldsymbol{m}$ with $m_0 \neq 0$ such that 2 but not 4 divides $|\boldsymbol{m}|^2$ are $(\pm 1, \pm 1, 0, 0)$ and permutations thereof, hence non trivial solutions are again only possible for $m_0 = 0$, and as before $\vec{r}$, $\vec{q}$ and $\vec{m}$ must be mutually orthogonal.

The last case to consider is $|\boldsymbol{r}|^2$ and $|\boldsymbol{q}|^2$ both even. Then $|\boldsymbol{m}|^2$ is an odd integer, but note that $\boldsymbol{m}$ may be half integral. Instead of (22) we consider again a weaker condition

$$2\boldsymbol{m} = -2y\boldsymbol{r} \bmod |\boldsymbol{m}|^2. \tag{27}$$

Everything is the same as before, except that here $\boldsymbol{m} = (\pm\frac{3}{2}, \pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2})$ are possible solutions. Of course it can only be a solution if $3\big||\boldsymbol{r}|^2$. Assume that $\boldsymbol{m} = (\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, which describes a rotation through the angle $\pi/3$, is a solution. Due to $\langle \boldsymbol{r}|\boldsymbol{m}\rangle = 0$ we have $\boldsymbol{r} = (0, r_1, r_2, -r_1 - r_2)$, which is equivalent to $(r_1 - r_2, r_1 + r_2, r_1 + r_2, r_1 + r_2)$.

Note that we have proved so far only that $\boldsymbol{m} = (\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ may be a solution of Eq. (22) if (and only if) $\boldsymbol{r} = (0, r_1, r_2, -r_1 - r_2)$ and $3\big||\boldsymbol{r}|^2 = 2(r_1^2 + r_2^2 + r_1 r_2)$. We have still to prove that Eq. (22) is indeed satisfied. Inserting $\boldsymbol{r}$ and $\boldsymbol{m}$ in Eq. (22) we obtain

$$\boldsymbol{n} = \frac{1}{|\boldsymbol{m}|^2}\bar{\boldsymbol{m}} + \frac{x}{|\boldsymbol{r}|^2}\bar{\boldsymbol{r}} = \frac{1}{6}(3,1,1,1) + \frac{x}{2(r_1^2 + r_2^2 + r_1 r_2)}(0, r_1, r_2, -r_1 - r_2) \tag{28}$$

and this is in fact a half integral quaternion if we choose $x = 2r_1(r_1^2 + r_2^2 + r_1 r_2)/3$ and take into account that $r_1 = r_2 \neq 0 \pmod 3$.

We can thus formulate the following lemma:

Lemma 3.6 *Let $\boldsymbol{r} = (0, r_1, r_2, r_3)$ and $\boldsymbol{q} = (0, q_1, q_2, q_3)$ be primitive. Then $Q = R(\boldsymbol{q})$ is a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$ if and only if one of the following conditions hold:*

- *Q is an element of the minimal symmetry group.*
- *There exists a (half)integral quaternion $\boldsymbol{m} = (0, m_1, m_2, m_3)$ such that $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$, i.e. there exists a (half)integral vector $\vec{m}$ such that $\vec{r} = \vec{q} \times \vec{m}$ and $\vec{q} \cdot \vec{m} = 0$.*
- *$\boldsymbol{r}$ is equivalent to $\boldsymbol{r}' = \boldsymbol{u}\boldsymbol{r}\boldsymbol{u}^{-1} = (0, r_1, r_2, -r_1 - r_2)$ and $\boldsymbol{r}' = 1/2\,\boldsymbol{u}\boldsymbol{q}\boldsymbol{u}^{-1}(3,1,1,1)$, i.e. $3\big||\boldsymbol{r}|^2$ and $\boldsymbol{q} = 1/6\,\boldsymbol{r}\boldsymbol{u}^{-1}(3,-1,-1,-1)\boldsymbol{u}$, where $\Sigma(\boldsymbol{u}) = 1$.*

Proof: We have already proved that it is necessary that one of these conditions holds. The first condition is sufficient by def. 3.1. From lemma 3.3 it follows immediately that the second condition is sufficient, too. Thus it remains to show that the third condition is sufficient. Let $\boldsymbol{r} = (0, r_1, r_2, -r_1 - r_2)$ and $3\big||\boldsymbol{r}|^2$. Then $r_1 = r_2 \pmod 3$ and hence $\boldsymbol{q} = 1/6\,\boldsymbol{r}(3,-1,-1,-1) = 1/3(0, r_1 - r_2, r_1 + 2r_2, -2r_1 - r_2)$ has integral components. Moreover $\boldsymbol{r}$ is equivalent to $1/2\,\boldsymbol{r}(1,-1,-1,-1) = 1/2\,\boldsymbol{q}(0,1,1,1) = -1/2\,(0,1,1,1)\boldsymbol{q}$, and again lemma 3.3 concludes the proof. $\square$

Note that $\boldsymbol{r} = (0, r_1, r_2, -r_1 - r_2)$ is equivalent to a quaternion of the form (m, n, n, n), and the last statement is equivalent to the fact that $R(0,1,1,1)$ and hence $R(3,1,1,1)$ are symmetry elements of the corresponding CSL if and only if 3 divides $\Sigma(R(m,n,n,n))$, i.e. $\boldsymbol{L}(R(m,n,n,n))$ has hexagonal symmetry if and only if 3 divides $\Sigma(R(m,n,n,n))$.

We can go a step further and ask how many ways there are to write $\boldsymbol{r}$ as a product of two vectorial quaternions $\boldsymbol{q} = (0, \vec{q})$ and $\boldsymbol{m} = (0, \vec{m})$ with $\Sigma(\boldsymbol{q})$ and $\Sigma(\boldsymbol{m})$ relatively prime. i.e., we want to determine the number of twofold rotation axes orthogonal to $\vec{r}$. Obviously to each decomposition $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$ there correspond two twofold rotation axes, namely $\vec{q}$ and $\vec{m}$, and to each decomposition $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$ there correspond the three additional decompositions $\boldsymbol{r} = (-\boldsymbol{q})(-\boldsymbol{m}) = -\boldsymbol{m}\boldsymbol{q} = \boldsymbol{m}(-\boldsymbol{q})$. If there are further decompositions, then there must exist additional twofold rotation axes orthogonal to $\vec{r}$. But this is impossible unless $\vec{r}$ is a fourfold or a sixfold rotation axis. If $\vec{r}$ is a fourfold axis, then $\Sigma(\boldsymbol{m}) = \Sigma(\boldsymbol{q})$, and hence $\Sigma(\boldsymbol{m}) = \Sigma(\boldsymbol{q}) = \Sigma(\boldsymbol{r}) = 1$, i.e. $\boldsymbol{r}$ is equivalent to $(0,1,0,0)$. Similarly if $\vec{r}$ is a sixfold rotation axis, then $\boldsymbol{r}$ must be equivalent to $(0,1,1,1)$, since $\Sigma(\boldsymbol{q}) = 3$ and $\Sigma(\boldsymbol{m}) = 1$ or vice versa. Thus, if a decomposition $\boldsymbol{r} = \boldsymbol{q}\boldsymbol{m}$ exists, it is unique up to trivial operations except for the two cases mentioned above.

With the knowledge we have developed so far we can immediately prove

Theorem 3.7 *Let $\boldsymbol{r}$ be equivalent to a vectorial quaternion $(0, r_1, r_2, r_3)$. Then the symmetry group of $\boldsymbol{L}(R(\boldsymbol{r}))$ is either the minimal symmetry group or the minimal symmetry group is a subgroup of it of order 2. In particular, we have (always $0 \neq n \neq m \neq 0$)*

1. *If $\boldsymbol{r} = (m, n, n, n)$ and 3 does not divide Σ, then the CSL has rhombohedral symmetry and its symmetry group is just the minimal symmetry group, generated by $3^+\ \ x, x, x$ and $R(0, n+m, n-m, -2n)$. There are precisely n_3 inequivalent CSLs for a fixed Σ.*
2. *If $\boldsymbol{r} = (m, n, n, n)$ and 3 divides Σ, then the CSL has hexagonal symmetry. If $\Sigma = 3$ the symmetry group is the minimal symmetry group generated by $R(3,1,1,1)$ and $R(0, 1-1, 0)$. If $\Sigma > 3$ the symmetry group is a proper supergroup of index 2 of the minimal symmetry group and is generated by $R(3,1,1,1)$ and $R(0, n+m, n-m, -2n)$. There are again n_3 inequivalent CSLs for a fixed Σ, except for $\Sigma = 3$, where we have only one.*

3. *If $\boldsymbol{r} = (m, n, 0, 0)$, the CSL has tetragonal symmetry, its symmetry group is the minimal symmetry group generated by $4^+ \quad x, 0, 0$ and $R(0, 0, m, n)$. There are n_2 inequivalent CSLs.*

4. *If $\boldsymbol{r} = (m, n, n, 0)$, the CSL has orthorhombic symmetry. Its symmetry group is again just the minimal symmetry group generated by $2 \quad x, x, 0$ and $R(0, n, -n, m)$. There are n_4 inequivalent CSLs.*

5. *If $\boldsymbol{r} = (0, \vec{r})$ is not equivalent to one of the cases above, then the CSL is orthorhombic if there exist two orthogonal integer vectors $\vec{q}$ and $\vec{m}$, $\vec{q}^2$ and $\vec{m}^2$ relatively prime, such that $\vec{r} = \vec{q} \times \vec{m}$ or $\vec{r} = 1/2\ \vec{q} \times \vec{m}$. This condition is equal to the existence of two integral quaternions $\boldsymbol{q}$, $\boldsymbol{m}$ such that $\boldsymbol{r} = 1/2^\ell \boldsymbol{q}\boldsymbol{m} = -1/2^\ell \boldsymbol{m}\boldsymbol{q}$. If no such decomposition exists then the CSL is monoclinic. The symmetry group of the former is generated by $R(0, \vec{r})$ and $R(0, \vec{q})$, whereas the latter is generated by $R(0, \vec{r})$. If Σ is a prime power, only the latter case is possible.*

These results are in coincidence with the observations of W. Grimmer [8], who has calculated the CSLs and there symmetries up to $\Sigma = 199$.

This theorem covers all CSLs where R is equivalent to a twofold operation. For the general case, only some partial answers exist. We want to discuss here only the question under what conditions $(0, r_1, r_2, r_3)$ describes a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$, $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$. We assume $r_0 \neq 0$, for otherwise the answer is trivial. Let $\boldsymbol{q} = 1/c(0, r_1, r_2, r_3)$, where c is the greatest common divisor of r_1, r_2, r_3. If $\boldsymbol{q}$ describes a symmetry operation, then $|\boldsymbol{q}|^2$ must divide $2|\boldsymbol{r}|^2$ and hence $2r_0^2$. From lemma 3.4 we infer that $1/|\boldsymbol{q}|^2 \bar{\boldsymbol{q}}\boldsymbol{r} = 1/|\boldsymbol{q}|^2(c|\boldsymbol{q}|^2, r_0\vec{q})$ must be a half integral quaternion, hence $|\boldsymbol{q}|^2$ must divide $2r_0$. Conversely, assume that $|\boldsymbol{q}|^2$ divides $2r_0$. Then $\boldsymbol{m} = 1/|\boldsymbol{q}|^2 \bar{\boldsymbol{q}}\boldsymbol{r}$ is a half integral quaternion, and since $\boldsymbol{q}$ and $\boldsymbol{r}$ commute it follows from lemma 3.3 that $\boldsymbol{q}$ corresponds to a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$. Thus we have proved

Lemma 3.8 *Let $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$, $\boldsymbol{q} = (1/c)(0, r_1, r_2, r_3)$, $c = \gcd(r_1, r_2, r_3)$. Then $R(\boldsymbol{q})$ is a symmetry operation of $\boldsymbol{L}(R(\boldsymbol{r}))$ if and only if $|\boldsymbol{q}|^2$ divides $2r_0$.*

For the special case $\boldsymbol{r} = (m, n, n, n)$ this lemma states that $(1, 1, 1)$ is a sixfold axis if and only if $\Sigma(\boldsymbol{r})$ is divisible by 3, a result that we have obtained previously by a different method.

4 Bravais lattices

So far we have only considered the symmetry of the CSLs, but we can go even further and compute the Bravais class of the CSL. For some CSLs the Bravais class follows immediately from theorem 3.7, e.g. for CSLs with hexagonal and rhombohedral symmetry we know at once that they must belong to the (unique) hexagonal and rhombohedral Bravais class, respectively. Consider now an orthorhombic CSL, then we cannot infer from symmetry to which of the four orthorhombic Bravais classes the CSL belongs. Nevertheless we can actually compute them.

As an example we consider an orthorhombic CSL generated by $\boldsymbol{r} = (0, \vec{r})$ such that $\vec{r} = \vec{q} \times \vec{m}$, where $\vec{q} \cdot \vec{m} = 0$ (case 5 of theorem 3.7). We assume further that $\vec{r}^2$, $\vec{q}^2$ and $\vec{m}^2$ are all odd. Then these three vectors are a basis for the CSL, since $\vec{q} \cdot \vec{r}^{(i)}/\vec{q}^2 = -m_i$ and $\vec{m} \cdot \vec{r}^{(i)}/\vec{m}^2 = q_i$ are integers and $|\vec{r}| \cdot |\vec{q}| \cdot |\vec{m}| = \vec{r}^2 = \Sigma(\boldsymbol{r})$. Hence the CSL is primitive orthorhombic.

Assume now that $\vec{r}^2$ and $\vec{q}^2$ are even, and hence $\vec{m}^2$ odd. Then $\vec{r}$, $\vec{q}$, $\vec{m}$ span a primitive orthorhombic sublattice of the CSL of index 2. Checking all combinations $\alpha_1\vec{r} + \alpha_2\vec{q} + \alpha_3\vec{m}$, $\alpha_i \in \{0, \pm 1/2\}$, we find that only the combinations $\pm 1/2\,(\vec{r} \pm \vec{q})$ are integral vectors, and hence the CSL must be C–face centered orthorhombic, with $1/2\,(\vec{r} \pm \vec{q})$, $\vec{m}$ as a possible basis.

Similarly one can discuss all the other cases. We finally find (for the conventions of the lattice parameters see [20]):

Theorem 4.1 *Let $\boldsymbol{r}$ be equivalent to $(0, \vec{r})$. Then $\boldsymbol{L}(R(\boldsymbol{r}))$ belongs to one of the following Bravais classes (always $0 \neq n \neq m \neq 0$):*

1. *If $\boldsymbol{r} \sim (m, n, n, n)$ and 3 does not divide Σ, then the CSL is rhombohedral with lattice parameters $a = \sqrt{2\Sigma}, c = \sqrt{3}$ (triple hexagonal setting).*

2. *If $\boldsymbol{r} \sim (m, n, n, n)$ and 3 divides Σ, then the CSL is hexagonal with lattice parameters $a = \sqrt{2\Sigma/3}, c = \sqrt{3}$.*

3. *If $\boldsymbol{r} \sim (m, n, 0, 0)$, the CSL is a primitive tetragonal lattice with lattice parameters $a = \sqrt{\Sigma}, c = 1$.*

4. *If $\boldsymbol{r} \sim (m, n, n, 0)$, the CSL is B–face centered orthorhombic with lattice parameters $a = \sqrt{2}, b = \sqrt{\Sigma}, c = \sqrt{2\Sigma}$.*

5. *If $\boldsymbol{r} = (0, \vec{r})$ is not equivalent to one of the cases above, and if there exist two orthogonal integer vectors $\vec{q}$ and $\vec{m}$, $\vec{q}^2$ and $\vec{m}^2$ relatively prime, such that $\vec{r} = \vec{q} \times \vec{m}$ or $\vec{r} = 1/2\ \vec{q} \times \vec{m}$, then the CSL is orthorhombic. In particular:*

(a) *If $\vec{r}^2$, $\vec{q}^2$ and $\vec{m}^2$ are all odd, the CSL is primitive orthorhombic with lattice parameters $a = |\vec{q}|$, $b = \sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}$.*

(b) *If $\vec{r}^2$ and $\vec{q}^2$ are even, then the CSL is B–face centered orthorhombic with lattice parameters $a = |\vec{q}|$, $b = \sqrt{2\Sigma}/|\vec{q}|$, $c = \sqrt{2\Sigma}$.*

(c) *If $\vec{r}^2$ is odd, $\vec{q}^2$ and $\vec{m}^2$ are even the CSL is C–face centered orthorhombic with lattice parameters $a = |\vec{q}|$, $b = 2\sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}$.*

6. *If $\boldsymbol{r} = (0, \vec{r})$ is not equivalent to one of the cases above, i.e. no decomposition $\vec{r} = 1/2^\ell \ \vec{q} \times \vec{m}$ exists, then the CSL is monoclinic. If $\vec{r}^2$ is odd, the CSL is primitive monoclinic; if $\vec{r}^2$ is even, the CSL is a C-type monoclinic lattice. If $\vec{r}$ is parallel to the c-axis then $c = \sqrt{\Sigma}$ in the first case and $c = \sqrt{2\Sigma}$ in the latter.*

5 Remarks on non–primitive cubic lattices

So far, we have only dealt with primitive cubic lattices, but many results remain true for face–centered and body–centered lattices, too. The index $\Sigma(R)$ and the number of equivalent and inequivalent CSLs are the same for all cubic lattices, and so is the symmetry of the CSLs [4, 7, 8].

The primitive cubic lattice $\boldsymbol{L}_p$ can be written as a union $\boldsymbol{L}_p = \boldsymbol{L}_0 \cup \boldsymbol{L}_1 \cup \boldsymbol{L}_2 \cup \boldsymbol{L}_3$ of four disjoint subsets of $\boldsymbol{L}_p$. Here $\boldsymbol{L}_i$ contains those vectors $\vec{v}$ of $\boldsymbol{L}_p$ for which $\vec{v}^2 = i \pmod 4$ holds. Note that only $\boldsymbol{L}_0 = 2\boldsymbol{L}_p$ is a lattice. Similarly we can write the body centered cubic lattice $\boldsymbol{L}_b$ and the face centered cubic lattice $\boldsymbol{L}_f$ as $\boldsymbol{L}_b = \boldsymbol{L}_0 \cup \boldsymbol{L}_1 \cup \boldsymbol{L}_2 \cup \boldsymbol{L}_3 \cup \frac{1}{2}\boldsymbol{L}_3 = \boldsymbol{L}_p \cup \frac{1}{2}\boldsymbol{L}_3$ and $\boldsymbol{L}_f = \boldsymbol{L}_0 \cup \boldsymbol{L}_1 \cup \boldsymbol{L}_2 \cup \boldsymbol{L}_3 \cup \frac{1}{2}\boldsymbol{L}_2 = \boldsymbol{L}_p \cup \frac{1}{2}\boldsymbol{L}_2$, respectively. One can show that $\boldsymbol{L}_p(R) \cap \boldsymbol{L}_i = \boldsymbol{L}_i \cap R\boldsymbol{L}_i =: \boldsymbol{L}_i(R)$, and hence $\boldsymbol{L}_b(R) = \boldsymbol{L}_p(R) \cup \frac{1}{2}\boldsymbol{L}_3(R)$ and $\boldsymbol{L}_f(R) = \boldsymbol{L}_p(R) \cup \frac{1}{2}\boldsymbol{L}_2(R)$, see e.g. [4]. These relations can then be used to prove that $\Sigma(R)$ is the same for all three types of cubic lattices, that the number of equivalent and inequivalent CSLs and their symmetry is the same for all cubic lattices as well.

Of course the lattices itself are different, and so the CSLs usually belong to different Bravais classes. First we generalize lemma 1.1 for body and face centered cubic lattices.

Lemma 5.1 *Let $\boldsymbol{L}_b$ be a body centered cubic lattice and $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$ a primitive quaternion. Then the CSL $\boldsymbol{L}_b(R(\boldsymbol{r}))$ is the $\mathbb{Z}$–span of the following vectors:*

- $\vec{r}^{(0)}, \vec{r}^{(1)}, \vec{r}^{(2)}, \vec{r}^{(3)}, 1/2\,(\vec{r}^{(0)} + \vec{r}^{(1)} + \vec{r}^{(2)} + \vec{r}^{(3)})$ *if $|\boldsymbol{r}|^2$ is odd,*
- $\vec{r}^{(0)}, 1/2\,(\vec{r}^{(0)} + \vec{r}^{(1)}), 1/2\,(\vec{r}^{(0)} + \vec{r}^{(2)}), 1/2\,(\vec{r}^{(0)} + \vec{r}^{(3)})$ *if $2 \big| |\boldsymbol{r}|^2$ and $4 \not\big| |\boldsymbol{r}|^2$,*
- $1/2\vec{r}^{(0)}, 1/2\vec{r}^{(1)}, 1/2\vec{r}^{(2)}, 1/2\vec{r}^{(3)}$ *if $4 \big| |\boldsymbol{r}|^2$.*

The situation is a bit nastier for the face centered lattice:

Lemma 5.2 *Let $\boldsymbol{L}_f$ be a face centered cubic lattice and $\boldsymbol{r} = (r_0, r_1, r_2, r_3)$ a primitive quaternion. Then we have the following cases:*

- *If $\boldsymbol{r}^2 = 3 \pmod 4$ define $\ell_i = 1$ if r_i is odd and $\ell_i = 0$ if r_i is even. Then $\boldsymbol{L}_f(R(\boldsymbol{r}))$ is the $\mathbb{Z}$–span of the vectors $2^{-\ell_0}\vec{r}^{(0)}, 2^{-\ell_1}\vec{r}^{(1)}, 2^{-\ell_2}\vec{r}^{(2)}, 2^{-\ell_3}\vec{r}^{(3)}$.*
- *If $\boldsymbol{r}^2 = 1 \pmod 4$ then $\boldsymbol{L}_f(R(\boldsymbol{r}))$ is the $\mathbb{Z}$–span of the vectors $\vec{r}^{(0)}, \vec{r}^{(1)}, \vec{r}^{(2)}, \vec{r}^{(3)}$ and those combinations $1/2\,(\vec{r}^{(i)} + \vec{r}^{(j)})$, for which $r_i + r_j$ is even.*
- *If $\boldsymbol{r}^2 = 2 \pmod 4$ define $\ell_i = 1$ if r_i is even and $\ell_i = 0$ if r_i is odd. Further define $m_i = 0$ if $1/2\,(r_0 - r_1 - r_2 - r_3) - r_i$ is even and $m_i = 1$ if $1/2\,(r_0 - r_1 - r_2 - r_3) - r_i$ is odd. Then $\boldsymbol{L}_f(R(\boldsymbol{r}))$ is the $\mathbb{Z}$–span of the vectors $2^{-\ell_i}\vec{r}^{(i)}$ and $2^{m_i}/4\,(\vec{r}^{(0)} + \vec{r}^{(1)} + \vec{r}^{(2)} + \vec{r}^{(3)} + 2\vec{r}^{(i)})$, $i = 0, \dots 3$.*
- *If $\boldsymbol{r}^2 = 0 \pmod 4$ then $\boldsymbol{L}_f(R(\boldsymbol{r}))$ is the $\mathbb{Z}$–span of the vectors $\vec{r}^{(0)}$, $1/4\,(\vec{r}^{(0)} + (-1)^{(r_0 - r_i)/2}\vec{r}^{(i)})$, $i = 1, 2, 3$.*

In principle one could use these representations to derive the symmetries and the Bravais class for the CSLs of the body and face centered cubic lattices. However, it is simpler to derive them from the primitive cubic case by means of $\boldsymbol{L}_b(R) = \boldsymbol{L}_p(R) \cup \frac{1}{2}\boldsymbol{L}_3(R)$ and $\boldsymbol{L}_f(R) = \boldsymbol{L}_p(R) \cup \frac{1}{2}\boldsymbol{L}_2(R)$. Finally we obtain the following results for the Bravais lattices. For the body centered case we have

Theorem 5.3 *Let $\boldsymbol{r}$ be equivalent to $(0, \vec{r})$. Then $\boldsymbol{L}_b(R(\boldsymbol{r}))$ belongs to one of the following Bravais classes (always $0 \neq n \neq m \neq 0$):*

1. *If $\boldsymbol{r} \sim (m, n, n, n)$ and 3 does not divide Σ, then the CSL is rhombohedral with lattice parameters $a = \sqrt{2\Sigma}, c = \sqrt{3}/2$ (triple hexagonal setting).*

2. *If $\boldsymbol{r} \sim (m,n,n,n)$ and 3 divides Σ, then the CSL is hexagonal with lattice parameters $a = \sqrt{2\Sigma/3}, c = \sqrt{3}/2$.*

3. *If $\boldsymbol{r} \sim (m,n,0,0)$, the CSL is a body centered tetragonal lattice with lattice parameters $a = \sqrt{\Sigma}, c = 1$.*

4. *If $\boldsymbol{r} \sim (m,n,n,0)$ with m odd and n even, then the CSL is face centered orthorhombic with lattice parameters $a = \sqrt{2}, b = \sqrt{\Sigma}, c = \sqrt{2\Sigma}$. If both m and n are odd then the CSL is a B–face centered orthorhombic lattice with lattice parameters $a = \sqrt{2}, b = \sqrt{\Sigma}/2, c = \sqrt{2\Sigma}$. If m is even and not divisible by 4, then the CSL is B–face centered orthorhombic with lattice parameters $a = \sqrt{2}, b = \sqrt{\Sigma}/2, c = \sqrt{2\Sigma}$. If m is divisible by 4, then the CSL is face centered orthorhombic with lattice parameters $a = \sqrt{2}, b = \sqrt{\Sigma}, c = \sqrt{2\Sigma}$.*

5. *If $\boldsymbol{r} = (0,\vec{r})$ is not equivalent to one of the cases above, and if there exist two orthogonal integer vectors $\vec{q}$ and $\vec{m}$, $\vec{q}^2$ and $\vec{m}^2$ relatively prime, such that $\vec{r} = \vec{q}\times\vec{m}$ or $\vec{r} = 1/2\,\vec{q}\times\vec{m}$, then the CSL is orthorhombic. In particular:*
   (a) *If $\vec{r}^2$, $\vec{q}^2$ and $\vec{m}^2$ are all odd, the CSL is body centered orthorhombic with lattice parameters $a = |\vec{q}|$, $b = \sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}$.*
   (b) *If $\vec{r}^2$ and $\vec{q}^2$ are even, then the CSL is B–face centered orthorhombic if $\vec{m} \in \boldsymbol{L}_3$ and face centered orthorhombic otherwise. The lattice parameters $a = |\vec{q}|$, $b = \sqrt{\Sigma}/2|\vec{q}|$, $c = \sqrt{2\Sigma}$ and $a = |\vec{q}|$, $b = \sqrt{2\Sigma}/|\vec{q}|$, $c = \sqrt{2\Sigma}$, respectively.*
   (c) *If $\vec{r}^2$ is odd, $\vec{q}^2$ and $\vec{m}^2$ are even, the CSL is C–face centered orthorhombic if $\vec{r} \in \boldsymbol{L}_3$ and face centered orthorhombic otherwise. The lattice parameters for these two cases read $a = |\vec{q}|$, $b = 2\sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}/2$ and $a = |\vec{q}|$, $b = 2\sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}$, respectively.*

6. *If $\boldsymbol{r} = (0,\vec{r})$ is not equivalent to one of the cases above, i.e. no decomposition $\vec{r} = 1/2^\ell\,\vec{q}\times\vec{m}$ with $\vec{q}\cdot\vec{m} = 0$ exists then the CSL is a C-type monoclinic lattice if $\vec{r}^2 \neq 3 \pmod 4$. If $\vec{r}^2 = 3 \pmod 4$ the CSL is primitive monoclinic.*

Similarly we can determine the Bravais classes in the face centered cubic case.

Theorem 5.4 *Let $\boldsymbol{r}$ be equivalent to $(0,\vec{r})$. Then $\boldsymbol{L}_f(R(\boldsymbol{r}))$ belongs to one of the following Bravais classes (always $0 \neq n \neq m \neq 0$):*

1. *If $\boldsymbol{r} \sim (m,n,n,n)$ and 3 does not divide Σ, then the CSL is rhombohedral with lattice parameters $a = \sqrt{\Sigma/2}, c = \sqrt{3}$ (triple hexagonal setting).*

2. *If $\boldsymbol{r} \sim (m,n,n,n)$ and 3 divides Σ, then the CSL is hexagonal with lattice parameters $a = \sqrt{\Sigma/6}, c = \sqrt{3}$.*

3. *If $\boldsymbol{r} \sim (m,n,0,0)$, the CSL is a body centered tetragonal lattice with lattice parameters $a = \sqrt{\Sigma/2}, c = 1$.*

4. *If $\boldsymbol{r} \sim (m,n,n,0)$ with m odd and n even, then the CSL is body centered orthorhombic with lattice parameters $a = 1/\sqrt{2}, b = \sqrt{\Sigma/2}, c = \sqrt{\Sigma}$. If both m and n are odd, then the CSL is a C–face centered orthorhombic lattice with lattice parameters $a = 1/\sqrt{2}, b = \sqrt{\Sigma/2}, c = \sqrt{\Sigma}$. If m is even and not divisible by 4 then the CSL is C–face centered orthorhombic lattice with lattice parameters $a = 1/\sqrt{2}, b = \sqrt{\Sigma/2}, c = \sqrt{\Sigma}$. If m is divisible by 4 the CSL is again a body centered orthorhombic lattice with lattice parameters $a = 1/\sqrt{2}, b = \sqrt{\Sigma/2}, c = \sqrt{\Sigma}$.*

5. *If $\boldsymbol{r} = (0,\vec{r})$ is not equivalent to one of the cases above, and if there exist two orthogonal integer vectors $\vec{q}$ and $\vec{m}$, $\vec{q}^2$ and $\vec{m}^2$ relatively prime, such that $\vec{r} = \vec{q}\times\vec{m}$ or $\vec{r} = 1/2\,\vec{q}\times\vec{m}$, then the CSL is orthorhombic. In particular:*
   (a) *If $\vec{r}^2$, $\vec{q}^2$ and $\vec{m}^2$ are all odd, the CSL is face centered orthorhombic with lattice parameters $a = |\vec{q}|$, $b = \sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}$.*
   (b) *If $\vec{r}^2$ and $\vec{q}^2$ are even, then the CSL is B–face centered orthorhombic with lattice parameters $a = |\vec{q}|/2$, $b = \sqrt{2\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma/2}$ if $1/2\,(\vec{r}+\vec{q}) \in \boldsymbol{L}_2$. If $1/2\,(\vec{r}+\vec{q}) \notin \boldsymbol{L}_2$ then $1/2\,(\vec{r}+\vec{q}) + \vec{m} \in \boldsymbol{L}_2$ and the CSL is body centered orthorhombic with lattice parameters $a = |\vec{q}|/2$, $b = \sqrt{2\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma/2}$.*
   (c) *If $\vec{r}^2$ is odd, $\vec{q}^2$ and $\vec{m}^2$ are even then the CSL is C–face centered orthorhombic or body centered orthorhombic, according to whether $1/2\,(\vec{q}+\vec{m}) \in \boldsymbol{L}_2$ or $1/2\,(\vec{q}+\vec{m})+\vec{r} \in \boldsymbol{L}_2$. In both cases the lattice parameters are $a = |\vec{q}|/2$, $b = \sqrt{\Sigma}/|\vec{q}|$, $c = \sqrt{\Sigma}$.*

6. *If $\boldsymbol{r} = (0,\vec{r})$ is not equivalent to one of the cases above, i.e. no decomposition $\vec{r} = 1/2^\ell\,\vec{q}\times\vec{m}$ with $\vec{q}\cdot\vec{m} = 0$ exists then the CSL is monoclinic. It is centered monoclinic except if $\vec{r}^2 = 3 \pmod 4$, where it is primitive monoclinic.*

Using these theorems one can immediately determine the Bravais class for each CSL $\boldsymbol{L}(R)$. Table 2 lists them for all CSLs with $\Sigma \leq 59$.

Σ	$\boldsymbol{r}$	CSL (cP)	CSL (cI)	CSL (cF)
3	$(0,1,1,1)$	hP	hP	hP
5	$(2,1,0,0)$	tP	tI	tI
7	$(2,1,1,1)$	hR	hR	hR
9	$(1,2,2,0)$	oC	oF	oI
11	$(3,1,1,0)$	oC	oC	oC
13	$(1,2,2,2)$	hR	hR	hR
13	$(3,2,0,0)$	tP	tI	tI
15	$(0,5,2,1)$	oC	oF	oI
17	$(4,1,0,0)$	tP	tI	tI
17	$(3,2,2,0)$	oC	oF	oI
19	$(4,1,1,1)$	hR	hR	hR
19	$(1,3,3,0)$	oC	oC	oC
21	$(3,2,2,2)$	hP	hP	hP
21	$(0,4,2,1)$	oC	oF	oI
23	$(0,6,3,1)$	mC	mC	mC
25	$(4,3,0,0)$	tP	tI	tI
25	$(0,5,4,3)$	mC	mC	mC
27	$(5,1,1,0)$	oC	oC	oC
27	$(0,7,2,1)$	mC	mC	mC
29	$(5,2,0,0)$	tP	tI	tI
29	$(0,4,3,2)$	mP	mC	mC
31	$(2,3,3,3)$	hR	hR	hR
31	$(0,7,3,2)$	mC	mC	mC
33	$(5,2,2,0)$	oC	oF	oI
33	$(1,4,4,0)$	oC	oF	oI
33	$(0,7,4,1)$	oC	oC	oC
35	$(0,5,3,1)$	oC	oC	oC
35	$(0,6,5,3)$	oC	oF	oI
37	$(6,1,0,0)$	tP	tI	tI
37	$(5,2,2,2)$	hR	hR	hR
37	$(0,8,3,1)$	mC	mC	mC
39	$(6,1,1,1)$	hP	hP	hP
39	$(5,3,2,1)$ $(-5,3,2,1)$	mC	mC	mC
41	$(5,4,0,0)$	tP	tI	tI
41	$(3,4,4,0)$	oC	oF	oI
41	$(0,6,2,1)$	mP	mC	mC
43	$(4,3,3,3)$	hR	hR	hR
43	$(5,3,3,0)$	oC	oC	oC
43	$(0,9,2,1)$	mC	mC	mC
45	$(0,5,4,2)$	oP	oI	oF
45	$(0,8,5,1)$	oC	oC	oC
45	$(0,7,5,4)$	oC	oC	oC
47	$(0,9,3,2)$	mC	mC	mC
47	$(0,7,6,3)$	mC	mC	mC
49	$(1,4,4,4)$	hR	hR	hR
49	$(0,6,3,2)$	mP	mC	mC
49	$(0,9,4,1)$	mC	mC	mC
51	$(7,1,1,0)$	oC	oC	oC
51	$(1,5,5,0)$	oC	oC	oC
51	$(5,4,3,1)$ $(-5,4,3,1)$	mP	mC	mC
53	$(7,2,0,0)$	tP	tI	tI
53	$(0,6,4,1)$	mP	mC	mC
53	$(0,9,4,3)$	mC	mC	mC
55	$(0,10,3,1)$	oC	oC	oC
55	$(0,9,5,2)$	mC	mC	mC
55	$(0,7,6,5)$	mC	mC	mC

Σ	$\boldsymbol{r}$	CSL (cP)	CSL (cI)	CSL (cF)
57	$(3,4,4,4)$	hP	hP	hP
57	$(7,2,2,0)$	oC	oF	oI
57	$(5,4,4,0)$	oC	oF	oI
57	$(6,4,2,1)$ $(-6,4,2,1)$	mC	mC	mC
59	$(3,5,5,0)$	oC	oC	oC
59	$(0,7,3,1)$	mP	mP	mP
59	$(0,9,6,1)$	mC	mC	mC

Table 2: Bravais classes of the CSLs with $\Sigma \leq 59$

6 Further remarks and outlook

We have derived the symmetry properties of the CSLs by making intensive use of quaternions and the proofs are mainly algebraic. A crystallographer not familiar with quaternions might be interested in a more geometric development of this topic. Indeed, one can prove most theorems with geometrical methods. We briefly sketch how this can be done for the primitive cubic case. Let $R = R(\boldsymbol{r}) = R(r_0, \vec{r})$ If $\vec{v} \in \boldsymbol{L}(R)$ then

$$R^{-1}\vec{v} = \frac{1}{r_0^2 + \vec{r}^2}\left((r_0^2 - \vec{r}^2)\vec{v} - 2r_0\vec{r}\times\vec{v} + 2(\vec{r}\cdot\vec{v})\vec{r}\right) \in \boldsymbol{L}, \tag{29}$$

i.e. $R^{-1}\vec{v}$ must be an integer vector. This expression simplifies if R is a rotation through π, where we have $r_0 = 0$. It then follows that $R^{-1}\vec{v} \in \boldsymbol{L}$ if and only if $\vec{r}^2$ divides $2\vec{r}\cdot\vec{v}$. If Q is a symmetry operation of $\boldsymbol{L}(R)$, then $Q^{-1}\vec{v} \in \boldsymbol{L}$ and $R^{-1}Q^{-1}\vec{v} \in \boldsymbol{L}$ for all $\vec{v} \in \boldsymbol{L}$. If we assume that Q is a rotation through π around the axis $\vec{q}$ we get the following two conditions: $\vec{q}^2$ must divide $2\vec{q}\cdot\vec{v}$ and

$$\frac{2\vec{q}\cdot\vec{v}}{\vec{q}^2}\left(-\vec{q} + \frac{2\vec{r}\cdot\vec{v}}{\vec{r}^2}\vec{r}\right) \in \boldsymbol{L}, \tag{30}$$

which implies that $\frac{2\vec{q}\cdot\vec{v}}{\vec{q}^2}\frac{2\vec{r}\cdot\vec{v}}{\vec{r}^2}$ is an integer. One shows further that there exist an integer n and an integer vector $\vec{c}$ orthogonal to $\vec{r}$ such that $\vec{r} = n\vec{q} + \vec{c}$ if $\vec{q}^2$ is odd and $\vec{r} = n/2\vec{q} + 1/2\vec{c}$ if $\vec{q}^2$ is even. Now one can prove that $\vec{r}^2$ must divide $4\vec{c}^2$. If $\vec{q}^2$ is even we have the stricter condition that $\vec{r}^2$ must divide $\vec{c}^2$. These conditions limit the possible values of n and $\vec{c}$. If one checks all the possible cases (which is a bit tedious) one finally arrives at theorem 4.1.

We have answered the question which symmetries a CSL has and to which Bravais class it belongs for all $\boldsymbol{r}$ equivalent to $(0, \vec{r})$, It would be interesting to answer the question also for the general case.

We have shown that a CSL has orthorhombic symmetry if $\boldsymbol{r}$ can be written as $2^\ell\boldsymbol{r} = \boldsymbol{qm} = -\boldsymbol{mq}$, or equivalently $\vec{r} = \vec{q}\times\vec{m}$, where $\vec{q}\cdot\vec{m} = 0$. Here the question arises under what conditions such a decomposition exists, and how many inequivalent decompositions exist for a given $\Sigma = 2^{-\ell}|\boldsymbol{r}|^2$. For a fixed $\boldsymbol{r}$, such a decomposition is unique up to sign changes and permutations, unless $\boldsymbol{r} \sim (0,1,1,1)$ or $(0,1,0,0)$. This question is related to the number of inequivalent but congruent CSLs. Grimmer suggests a formula relating the number of congruent CSLs with several other properties like the symmetry of the CSL[8]. This formula is based on the analysis of the CSLs up to $\Sigma = 199$. Using our results, this formula can be proved for the hexagonal, tetragonal and rhombohedral CSLs. For the orthorhombic case, one would need a formula for the number of representations of the kind $2^m\boldsymbol{r} = \boldsymbol{qm} = -\boldsymbol{mq}$.

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